

Anion size dependence of band gaps of iodido antimonates

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Halogenido complexes of heavy group 15 elements show promising semiconductor properties that make them interesting as substituents for their excellently performing but also toxic lead counterparts.[1] However, especially the family of iodido antimonates is quite scarcely investigated and the literature even states somewhat contradicting information with regard to the optical band gaps of these compounds. For example, the published band gaps for compounds featuring the one dimensional $[\text{SbI}_5]^{2-}$ -anion reach from 1.79 eV [2] up to 2.41 eV [3], although data of closely related bismuth compounds suggests, that this range should be much smaller.[4]

We recently were able to synthesize $[\text{Hpyz}]_4[\text{Sb}_{10}\text{I}_{34}]$ (pyz = pyrazine, $\text{N}_2\text{C}_4\text{H}_4$), which features the largest discrete halogenido pentelate anion yet. Its structural motif can be understood as a cut out from the CdI_2 -structure. This motif is quite common for iodido antimonates and ions of this type with the general formula $[\text{Sb}_{2n}\text{I}_{3n+4}]^{4-}$ are known for $n = 1 - 5$. [5-7] With this series of compounds at hand we decided to investigate the influence of the anion size on the optical band gap by experimental and theoretical means to shed some more light on the electronic structure of iodido antimonates close to the absorption edge.

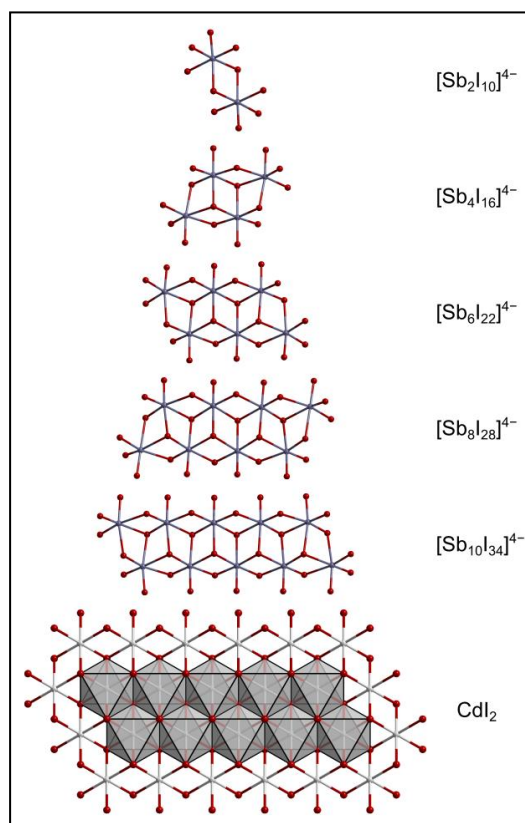


Fig. 1: Structural motifs of iodido antimonates derived from the CdI_2 structure.[5-7]

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